

9,21-dimethyl-pentatriacontane

Inchi:	InChI=1S/C37H76/c1-5-7-9-11-13-14-15-16-18-21-25-29-34-37(4)35-31-27-23-20-17-19
InchiKey:	IYIGCCPWMKNTDI-UHFFFAOYSA-N
Formula:	C37H76
SMILES:	CCCCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CCCCCCCC
Mol. weight [g/mol]:	521.00

Physical Properties

Property code	Value	Unit	Source
gf	255.78	kJ/mol	Joback Method
hf	-817.57	kJ/mol	Joback Method
hfus	84.54	kJ/mol	Joback Method
hvap	97.18	kJ/mol	Joback Method
log10ws	-14.83		Crippen Method
logp	14.391		Crippen Method
mcvol	532.190	ml/mol	McGowan Method
pc	442.47	kPa	Joback Method
rinpol	3561.00		NIST Webbook
rinpol	3561.00		NIST Webbook
rinpol	3563.00		NIST Webbook
rinpol	3561.00		NIST Webbook
rinpol	3563.00		NIST Webbook
tb	1045.08	K	Joback Method
tc	1340.34	K	Joback Method
tf	476.75	K	Joback Method
vc	2.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1965.02	J/molxK	1045.08	Joback Method
cpg	2001.02	J/molxK	1094.29	Joback Method
cpg	2034.16	J/molxK	1143.50	Joback Method
cpg	2064.75	J/molxK	1192.71	Joback Method
cpg	2093.10	J/molxK	1241.92	Joback Method

cpg	2119.51	J/molxK	1291.13	Joback Method
cpg	2144.28	J/molxK	1340.34	Joback Method
dvisc	0.0005532	Paxs	476.75	Joback Method
dvisc	0.0001441	Paxs	571.47	Joback Method
dvisc	0.0000550	Paxs	666.19	Joback Method
dvisc	0.0000267	Paxs	760.91	Joback Method
dvisc	0.0000152	Paxs	855.64	Joback Method
dvisc	0.0000097	Paxs	950.36	Joback Method
dvisc	0.0000067	Paxs	1045.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R300653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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